Journal of Hydrology 532 (2016) 37–45

Contents lists available at ScienceDirect

Journal of Hydrology

journal homepage: www.elsevier.com/locate/jhydrol

Additional longitudinal displacement for contaminant dispersion in wetland flow

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ARTICLE INFO

Article history:
Received 13 August 2015
Received in revised form 25 October 2015
Accepted 26 October 2015
Available online 3 November 2015
This manuscript was handled by Geoff Syme, Editor-in-Chief

Keywords:
Taylor dispersion
Point source
Wetland flow
Longitudinal displacement
Vertical concentration distribution

SUMMARY

When there is a sudden and uniform release of contaminant over the depth of wetland, the centroid of resulted solute cloud will travel downstream at the cross-sectional mean velocity of the flow. However, if the initial release is not uniform, there will be an additional longitudinal displacement of the centroid, which is important for predicting the concentration distribution but cannot be revealed by the classical one-dimensional Taylor dispersion model. For the most typical case of an initial point source release at the free-water-surface of the wetland, an idealized case modeling accidental leakage of toxic chemicals in waters, in the present paper we analytically deduce the longitudinal displacement by the method of concentration moment. The result is then incorporated in the analytical solutions of concentration distribution, which are further verified by our numerical simulations. The effects of the longitudinal displacement on the concentration distribution are analyzed in detail. It is shown that without considering the displacement, for vertical planes close to the edges of the contaminant cloud, the analytical solution can over- or under-estimate the vertical distribution of concentration for over 20% of the maximum concentration in the plane even at a large dimensionless time of $t^* = 5$. The longitudinal displacement is shown to decrease with the increase of the important damping factor α, which characterizes the effects of vegetation in wetlands. A simple application is given at the end of this paper to illustrate the evolution of the additional longitudinal displacement.

1. Introduction

Contaminant transport in wetland flow has attracted intensive research efforts in recent years for its essential implications in the field of environmental science and engineering; and related applications include environmental risk assessment, wastewater treatment and ecological restoration (Fischer, 1976; Fischer et al., 1979; Guerrero and Skaggs, 2010; Larsen et al., 2009; Murphy et al., 2007; Ngo-Cong et al., 2015; Pannone, 2014; Shao and Chen, 2013; Wu and Chen, 2014a; Wu et al., 2011a, 2015; Yuan et al., 2013). For understanding the asymptotic contaminant concentration evolution in wetland flow, Taylor dispersion is a concept of fundamental importance (Taylor, 1953, 1954; Wu et al., 2015).

Generally, Taylor dispersion (Taylor, 1953) refers to a stage of the transport process after the initial injection of the contaminant, during which the centroid of the contaminant cloud moves downstream with the transverse mean velocity of the flow, while at the same time the longitudinal distribution of the mean concentration can be described by a one-dimensional diffusion equation (known as the Taylor dispersion model). Because the Taylor diffusion coefficient in the diffusion equation can be several orders of magnitude greater than the molecular diffusion coefficient (or similar effective coefficient in the governing convection–diffusion equation for the transport, like turbulent diffusion coefficient (Taylor, 1954)), the contaminant cloud disperses much faster than its diffusion in standing water (or transversely uniform flow). Since Taylor's initiative, extensive studies have focused on the accurate prediction of the mean concentration distribution during the transport, both analytically and numerically (Chatwin, 1970; Gill and Sankarasubramanian, 1970; Houseworth, 1984; Latini and Bernoff, 2001; Phillips and Kaye, 1996; Ratnakar and Balakotaiah, 2011; Smith, 1981; Stokes and Barton, 1990; Wu and Chen, 2014b). Recently, there are also efforts in characterizing the multi-dimensional concentration distribution (Wu and Chen, 2014a; Wu et al., 2015), indicating a highly non-uniform transverse concentration distribution when Taylor dispersion model is applicable, which can last for a very long period of time, in contrast to the traditional view of a uniform transverse distribution for Taylor dispersion process (Latini and Bernoff, 2001; Stokes and Barton, 1990; Taylor, 1953).

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http://dx.doi.org/10.1016/j.jhydrol.2015.10.064
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For progress in the analytical study of contaminant transport in wetland flow, different approaches including the method of concentration moment (Chen et al., 2012; Wu et al., 2012; Zeng et al., 2014), the homogenization technique (Ng, 2000; Ng and Bai, 2005; Wu et al., 2011b), and the method of mean concentration expansion (Chen, 2013) have been applied to determine the Taylor dispersion coefficient of the process. The discussed configurations of the wetland flow region range from the originally considered single zone with homogeneous media (such as the granular material or vegetation) (Zeng, 2010), to the extended multi-zone structure (Wang et al., 2013; Wu et al., 2011a) taking into account the effect of transverse media distribution heterogeneity, which is a typical case for both natural and constructed wetlands. The theoretical foundation enabling these analytical explorations by methods for pure fluid flows is the application of the theory of phase-average (Liu and Masliyah, 2005; Wu et al., 2015). The complicated or even unknown flow and mass transfer details at the stem-scale caused by the existence of vegetation (for example) in wetlands will be removed by the phase-average operation performed at an intermediate scale which is greater than the stem-scale but smaller than the macro-scale as characterized by the height or width of the wetland channel (Liu and Masliyah, 2005; Zeng, 2010), resulting in continuous distributions for both flow and contaminant concentration.

All the studies mentioned above have mainly focused on analyzing the Taylor dispersion coefficient, and the initial condition of an uniform and instantaneous contaminant release over the cross-section of the wetland channel have been adopted. It is well known that for long time evolution, the Taylor dispersion coefficient will not depend on the initial condition of the transport process; however, the longitudinal distribution of the mean contaminant concentration will be affected by different initial conditions in some ways (Aris, 1956; Houseworth, 1984). For the previously considered line-source release (for the two-dimensional configuration of the wetland), during the entire transport process the centroid of the contaminant cloud remains at the origin of the coordinate system which moves downstream with the transverse mean velocity of the flow (Wu et al., 2015). But for the initial release of a point-source at the free-water-surface of the wetland, which is a most typical case in environmental risk assessment as encountered in the leakage of toxic chemicals in waters (Fischer et al., 1979), the centroid of the contaminant can initially move faster than the mean flow velocity, and then approaches the mean velocity gradually (Aris, 1956). Thus, when the contaminant transport finally enters the Taylor dispersion stage, there will be an additional longitudinal displacement compared with that of the previous case. Without taking into consideration this additional displacement, there will be added errors introduced in the prediction of the contaminant concentration. However, the important questions on how the additional displacement will affect the concentration distribution, and how to modify the analytical solution for contaminant dispersion of a point-source in wetland flow, have never been addressed.

In this paper, for the typical case of an initial contaminant release at the free-water-surface of the wetland flow, we analytically deduced the longitudinal displacement of contaminant dispersion by the method of concentration moment. After introducing the basic equation for contaminant transport at the beginning of part 2, we successively solve corresponding moment equations to determine the zero-th and first-order moments, which are used for the desired additional displacement and Taylor dispersion coefficient. The analytical solutions for the concentration distribution with and without incorporating the displacement are respectively given. The effects of the displacement are analyzed in detail by the analytical and new numerical results in part 3. Some conclusions are summarized at the end of this paper.

2. Methods and materials

For the case of an uniform release of contaminant over the depth of wetlands, the solute will be carried downstream by different velocities of the flow at different vertical positions right after the injection. It has been mathematically deduced (Aris, 1956; Wu et al., 2011a, 2012) that the centroid of the resulted contaminant cloud can move exactly with the vertical mean velocity of the flow for all the time, although the longitudinal distribution of the mean concentration is far from Gaussian at the very beginning of the transport. Alternatively, if the initial condition is a point source release at the free-water-surface of the wetland as to be discussed in this paper, this point contaminant will be immediately carried downstream by the fastest flow velocity at the water surface, while at the same time reaches the lower vertical position by molecular diffusion and travels with a slower speed. Thus, for the pre-stage of Taylor dispersion, the velocity of the contaminant cloud centroid under this different initial condition will have a greater value than the mean flow velocity, although the difference will decrease with time and approach zero in Taylor dispersion process.

A sketch is given as Fig. 1 to illustrate the configuration of the wetland channel with a depth of H. In a Cartesian coordinate system, x-axis defines the longitudinal direction, z-axis defines the vertical direction, and origin O is set at the channel bed wall.

Under the framework of phase-average, the general mass transfer equation can be adopted for contaminant transport in wetland as (Liu and Masliyah, 2005; Wu et al., 2015; Zeng, 2010):

$$\phi\frac{\partial C}{\partial t} + \nabla\cdot(\mathbf{U}C) = \nabla\cdot(\kappa\lambda\phi\nabla C) + \kappa\nabla\cdot(\mathbf{K}\cdot\nabla C), \tag{1}$$

where ϕ is the porosity, C the concentration, t the time, $\mathbf{U}$ the velocity, κ the tortuosity, λ the concentration diffusion coefficient, and $\mathbf{K}$ concentration dispersivity tensor.

For the most idealized case of homogeneous wetlands with constant parameters, Eq. (1) is simplified into (Chen, 2013; Zeng, 2010)

$$\frac{\partial C}{\partial t} + \frac{u}{\phi}\frac{\partial C}{\partial x} = \kappa\left(\lambda + \frac{K}{\phi}\right)\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial z^2}\right), \tag{2}$$

where u is the longitudinal velocity as a function of z, K is the concentration dispersivity.

The initial condition of a point-source release with mass Q at the free-water-surface is

$$C(x,z,t)|_{t=0} = Q\ \delta(x)\ \delta(H-z), \tag{3}$$

where $\delta(\cdot)$ is the Dirac-delta function.

The boundary conditions can be given as:

$$\left.\frac{\partial C}{\partial z}\right|_{z=0} = \left.\frac{\partial C}{\partial z}\right|_{z=H} = 0, \tag{4}$$

$$C(x,z,t)|_{x=\pm\infty} = 0. \tag{5}$$

Introducing the following dimensionless parameters:

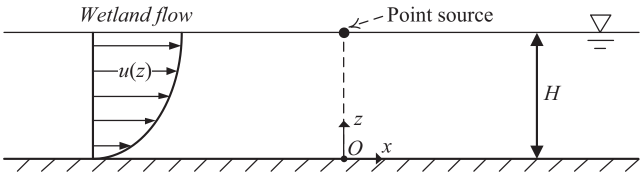

Fig. 1. Sketch for the instantaneous point release at free-water-surface of the wetland.